

Exact dimer ground states for a continuous family of quantum spin chains

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Abstract

Using the matrix product formalism, we define a multi-parameter family of spin models on one dimensional chains, with nearest and next-nearest neighbor anti-ferromagnetic interaction for which exact analytical expressions can be found for its doubly degenerate ground states. The family of Hamiltonians which we define, depend on 5 continuous parameters and the Majumdar-Ghosh model is a particular point in this parameter space. Like the Majumdar-Ghosh model, the doubly degenerate ground states of our models have a very simple structure, they are the product of entangled (dimer) states on adjacent sites. In each of these states there is a non-zero staggered magnetization, which vanishes when we take their translation-invariant combination as the new ground states. At the Majumdar-Ghosh point, these entangled states become the spin-singlets pertaining to this model. We will also calculate in closed form the two point correlation functions, both for finite size of the chain and in the thermodynamic limit.

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1 Introduction

One of the basic problems of many body physics is to use analytical and numerical tools to find the ground state of a many-body system governed by a given Hamiltonian. Unfortunately, except for a few exactly solvable examples, the task of finding the exact ground state of a given Hamiltonian is notoriously difficult. Moreover in some cases also like the anti-ferromagnetic Heisenberg chain, although the ground state is known, its structure turns out to be quite complicated, making the calculation of correlation functions very difficult.

In dealing with difficult problems, one way round the difficulty is to investigate the inverse problem, that is to start from states with pre-determined properties and find the family of Hamiltonians for which such a state is an exact ground state. The suitable formalism for following this path is the matrix product formalism, which was first realized in the work of [1], then formalized in finitely correlated states [2, 3], also known as optimal [4, 5] or matrix product states. This formalism has been followed in recent years both constructing various models of interacting spins on chains, [4, 5], ladders [6, 7] and some two dimensional lattices [8].

It has also been studied to gain a better understanding of many phenomena in correlated systems, i.e. quantum phase transitions [9], renormalization group algorithms [10], and entanglement [11].

Of particular interest to us in this paper is the so called Majumdar-Ghosh model defined on a ring of $2N$ sites by the following Hamiltonian

$$H_0 = \sum_{i=1}^{2N} 2\sigma_i \cdot \sigma_{i+1} + \sigma_i \cdot \sigma_{i+2}, \quad (1)$$

which has been introduced and solved exactly in a series of papers long ago [12, 13, 14], before the advent of the matrix product formalism, and later found to have a matrix product representation [15]. It was shown in the original papers that the ground state of this system is doubly degenerate, and each of these states has a very simple structure, that is, it is a product of singlets on adjacent sites. Let us call these ground states $|\phi_1\rangle$ and $|\phi_2\rangle$, and denote a singlet state on two adjacent sites by $S = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$, where $|0\rangle$ and $|1\rangle$ denote the up and down spin in the z direction, i.e. $|0\rangle = |z,+\rangle$, $|1\rangle = |z,-\rangle$. Then the degenerate ground states of (1) are:

$$\begin{aligned} |\phi_1\rangle &= S_{1,2} S_{3,4} \cdots S_{2N-1,2N}, \\ |\phi_2\rangle &= S_{2N,1} S_{2,3} \cdots S_{2N-2,2N-1}, \end{aligned} \quad (2)$$

with $H_0|\phi_{1,2}\rangle = -6N|\phi_{1,2}\rangle$. From these two states, one can form the new states $|\Psi_\pm\rangle := |\phi_1\rangle \pm |\phi_2\rangle$, which are eigenstates of the single-unit translation operator T on the ring, i.e. $T|\Psi_\pm\rangle = \pm|\Psi_\pm\rangle$. The correlation functions on these new translation invariant ground states, denoted by the subscripts \pm , are defined as:

$$\langle \sigma_1^a \sigma_r^a \rangle_\pm = \frac{\langle \Psi_0^\pm | \sigma_1^a \sigma_r^a | \Psi_0^\pm \rangle}{\langle \Psi_0^\pm | \Psi_0^\pm \rangle}, \quad a = x, y, z.$$

These were calculated in thermodynamic limit ($N \rightarrow \infty$) in [12] and were found to be

$$\langle \sigma_1^a \sigma_r^a \rangle_{\pm} = -\frac{1}{2} \delta_{r,2} \quad a = x, y, z. \quad (3)$$

Since then many works have been done on different aspects of this model[16], including studies of spontaneous dimereization, excitation spectrum [17] and renormalization group study [18] of this or very closely related models (i.e. models with anisotropy). It has also been shown [19] that the Majumdar-Ghosh model is the first member of a discrete series of models, all having exact dimer ground states, where exchange coupling decreases linearly with the separation of spins, and vanishes beyond a certain range, ν ($\nu = 2$ for the Majumdar-Ghosh model).

The aim of this paper is to study the Majumdar Ghosh model in the context of matrix product formalism and in this way introduce a multi-parameter deformations of this model and prove that its ground state is still doubly degenerate and dimerized. As is clear from (1), the Majumdar-Ghosh model is rotationally invariant. What we will do in this paper is that we reduce this symmetry to rotations in the $x - y$ plane only and ask what are the Hamiltonians on the chain with nearest and next-nearest neighbor interactions, which are still exactly solvable.

We will find a multi-parameter family of such exactly solvable Hamiltonians and show that their ground states are doubly degenerate and of dimer type. Both the Hamiltonian and their ground states will reduce to those of the Majumdar-Ghosh model in a certain limit. We will calculate all the correlation functions not only in thermodynamic limit, but for any finite N . Our generalization of this model may shed light on some aspects of the Majumdar-Ghosh model and provide different proofs for some of its properties.

Moreover, since the model is less symmetric and has 5 tunable parameters, it may be more flexible for matching with real experimental situations.

The structure of this paper is as follows: first we review briefly the matrix product formalism in section (2) and then in section (3) we derive the Majumdar-Ghosh model by using the matrix product formalism. In section (4) we use the same formalism to construct a continuous multi-parameter family of models, and show that the original Majumdar-Ghosh model corresponds to a specific point in this parameter space. In various subsections of this section we make a detailed study of this model, derive its Hamiltonian, determine the structure of its ground state and prove that the doubly degenerate ground states of this model have a simple structure, that is, they are products of entangled spin states on adjacent sites, in the same way that the ground states of the Majumdar-Ghosh model are products of singlets on adjacent sites. We also calculate all the one and the two point- functions of this model. In particular we show that each of the degenerate ground states has a non-zero staggered magnetization, however the translation-invariant ground states have zero staggered magnetization. We conclude the paper with a discussion.

2 Matrix Product States

Let us first make a quick review of the matrix product states in a language which we find convenient [9]. For more detailed reviews of the subject, the reader can consult more comprehensive review articles [15]. Consider a ring of N sites, where each site describes a d -level state. The Hilbert space of each site is spanned by the basis vectors $|i\rangle$, $i = 0, \dots, d - 1$. A state

$$|\Psi\rangle = \sum_{i_1, i_2, \dots, i_N} \Psi_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$

is called a matrix product state if there exist matrices A_i , $i = 0, \dots, d - 1$ (of dimension D), such that

$$\Psi_{i_1 i_2 \dots i_N} = \frac{1}{\sqrt{Z}} \text{tr}(A_{i_1} A_{i_2} \dots A_{i_N}), \quad (4)$$

where Z is a normalization constant. This constant is given by

$$Z = \text{tr}(E^N),$$

where

$$E = \sum_{i=0}^{d-1} A_i^* \otimes A_i.$$

Note that we are here considering homogeneous matrix product states (MPS) where the matrices depend on the value of the spin at each site and not on the site itself. More general MPS's can be defined where the matrices depend also on the sites [15]. It has been shown that such states can represent any quantum state on a chain [?].

The collection of matrices $\{A_i\}$ and $\{\mu U A_i U^{-1}\}$, where μ is an arbitrary complex number, both lead to the same matrix product state, the freedom in scaling with μ , is due to its cancelation with Z in the denominator of (4). This freedom will be useful when we discuss symmetries.

Symmetries: The state $|\Psi\rangle$ is reflection symmetric if there exists a matrix Π and a scalar σ such that

$$A_i^T = \sigma \Pi A_i \Pi^{-1} \quad \forall i.$$

It is invariant under spin flip transformation if there exists a matrix X and a scalar λ , such that

$$A_{\bar{i}} = \lambda X A_i X^{-1} \quad \forall i.$$

Finally, it is time-reversal invariant if there exists a matrix V , and a scalar τ such that

$$A_i^* = \tau V A_i V^{-1}, \quad \forall i.$$

In this article, we work with real matrices so that the last condition is automatically satisfied. Let us now turn to continuous symmetries.

Consider a local symmetry operator R acting on a site as $R|i\rangle = R_{ji}|j\rangle$ where summation convention is being used. R is a d dimensional unitary representation of the symmetry. A global symmetry operator $\mathcal{R} := R^{\otimes N}$ will then change this state to another matrix product state

$$\Psi_{i_1 i_2 \dots i_N} \longrightarrow \Psi'_{i_1 i_2 \dots i_N} := \text{tr}(A'_{i_1} A'_{i_2} \cdots A'_{i_N}),$$

where

$$A'_i := R_{ij} A_j.$$

The state $|\Psi\rangle$ is invariant under this symmetry if there exist an operator $U(R)$ and a scalar λ_R such that

$$R_{ij} A_j = \lambda_R U^{-1}(R) A_i U(R). \quad (5)$$

Repeating this transformation puts the constraint

$$\lambda_{R'} \lambda_R U_{R'} U_R = \lambda_{R'R} U_{R'R}.$$

Thus $U(R)$ is a D dimensional *projective* representation of the symmetry R . In case that R is a continuous symmetry with generators T_a , equation (5), leads to

$$(T_a)_{ij} A_j = [A_i, T_a] + \mu_a A_i, \quad (6)$$

where T_a and \mathcal{T}_a are the d - and D -dimensional representations of the Lie algebra of the symmetry, and μ_a are numbers. In this paper we will restrict our study to the case of $\mu_a = 0$. Equations (5) and (6) will be our guiding lines in defining states with prescribed symmetries.

The Hamiltonian: Given a matrix product state, the reduced density matrix of one site is given by

$$\rho_{ij} = \frac{\text{tr}((A_i^* \otimes A_j) E^{N-1})}{\text{tr}(E^N)}.$$

This density matrix has at least $d - D^2$ zero eigenvalues. To see this, suppose that we can find complex numbers c_j such that

$$\sum_{j=0}^{d-1} c_j A_j = 0. \quad (7)$$

This is a system of D^2 equations for d unknowns which has at least $d - D^2$ independent solutions. Any solution c_j gives a null eigenvector of ρ_{ij} . Thus the null space of the reduced density matrix of one site comprises a subspace of at least $d - D^2$ dimension, spanned by the independent solutions of equation (7).

The same reasoning applies to reduced density matrices of k consecutive sites which are given by

$$\rho_{i_1 \dots i_k, j_1 \dots j_k} = \frac{\text{tr}((A_{i_1}^* \cdots A_{i_k}^* \otimes A_{j_1} \cdots A_{j_k}) E^{N-k})}{\text{tr}(E^N)}.$$

In this case the null space of the reduced density matrix of k sites is spanned by the solutions of

$$\sum_{j_1, \dots, j_k=0}^{d-1} c_{j_1 \dots j_k} A_{j_1} \cdots A_{j_k} = 0. \quad (8)$$

The number of independent solutions of this system of equation is now $d^k - D^2$. Thus for the density matrix of k sites to have a null space it is sufficient (but not necessary and this is a crucial point) that the following inequality holds

$$d^k > D^2.$$

Let the null space of the reduced density matrix be spanned by the orthogonal vectors $|e_\alpha\rangle$, ($\alpha = 1, \dots, s \geq d^k - D^2$). Then we can construct the local hamiltonian acting on k consecutive sites as

$$h := \sum_{\alpha=1}^s \lambda_\alpha |e_\alpha\rangle\langle e_\alpha|,$$

where λ_α 's are positive constants. These constants together with the parameters of the vectors $|e_\alpha\rangle$ inherited from those of the original matrices A_i , determine the total number of coupling constants of the Hamiltonian. If we call the embedding of this local Hamiltonian into the sites l to $l+k$ by $h_{l,l+k}$ then the full Hamiltonian on the chain is written as

$$H = \sum_{l=1}^N h_{l,l+k}.$$

The state $|\Psi\rangle$ is then a ground state of this hamiltonian with vanishing energy. The reason is as follows:

$$\langle \Psi | H | \Psi \rangle = \text{tr}(H|\Psi\rangle\langle \Psi|) = \sum_{l=1}^N \text{tr}(h_{l,l+k}\rho_{l,l+k}) = 0,$$

where $\rho_{l,k+l}$ is the reduced density matrix of sites l to $l+k$ and in the last line we have used the fact that h is constructed from the null eigenvectors of ρ for k consecutive sites. Given that H is a positive operator, this proves the assertion.

Correlation functions: Let O be any local operator acting on a single site. Then we can obtain the one point function on site k of the chain $\langle \Psi | O(k) | \Psi \rangle$ as follows:

$$\langle \Psi | O(k) | \Psi \rangle = \frac{\text{tr}(E^{k-1} E_O E^{N-k})}{\text{tr}(E^N)}, \quad (9)$$

where

$$E_O := \sum_{i,j=0}^{d-1} \langle i | O | j \rangle A_i^* \otimes A_j.$$

In the thermodynamic limit $N \rightarrow \infty$, equation (9) gives

$$\langle \Psi | O | \Psi \rangle = \frac{\langle \lambda_{\max} | E_O | \lambda_{\max} \rangle}{\lambda_{\max}}$$

where we have used the translation invariance of the model and λ_{max} is the eigenvalue of E with the largest absolute value, for which the matrix element is non-vanishing, and $|\lambda_{max}\rangle$ and $\langle\lambda_{max}|$ are the right and left eigenvectors corresponding to this eigenvalue, normalized such that $\langle\lambda_{max}|\lambda_{max}\rangle = 1$. Here we are assuming that the largest eigenvalue of E is non-degenerate.

The n-point functions can be obtained in a similar way. For example, the two-point function $\langle\Psi|O(k)O(l)|\Psi\rangle$ can be obtained as

$$\langle\Psi|O(k)O(l)|\Psi\rangle = \frac{tr(E_O(k)E_O(l)E^N)}{tr(E^N)} \quad (10)$$

where $E_O(k) := E^{k-1}E_OE^{-k}$. Note that this is a formal notation which allows us to write the n-point functions in a uniform way, it does not require that E is an invertible matrix. In the thermodynamic limit the two point function turns out to be

$$\langle\Psi|O(1)O(r)|\Psi\rangle = \frac{1}{\lambda_{max}^{r-2}} \sum_i \lambda_i^{r-2} \langle\lambda_{max}|E_O|\lambda_i\rangle \langle\lambda_i|E_O|\lambda_{max}\rangle.$$

3 The Majumdar-Ghosh model

We take the size of the ring an even number $2N$. Let us also choose $d = 2$ (spin 1/2 particles), $k = 3$ (interactions up to next-nearest neighbors) and work with $D = 3$ dimensional matrices. Note that the condition $d^k > D^2$ is not satisfied here, but in view of the fact that this is a sufficient and not necessary condition, this will not be a source of concern. The basic symmetry that we demand is the rotational symmetry around the z axis, which according to (6) demands that there be a matrix S_z such that

$$[A_0, S_z] = \frac{1}{2}A_0, \quad [A_1, S_z] = -\frac{1}{2}A_1.$$

Working in a basis where $S_z = \text{diagonal}(-1/2, 0, 1/2)$, these equations immediately show that A_0 and A_1 should be of the following form:

$$A_0 := \begin{pmatrix} 0 & p & 0 \\ 0 & 0 & q \\ 0 & 0 & 0 \end{pmatrix}, \quad A_1 := \begin{pmatrix} 0 & 0 & 0 \\ h & 0 & 0 \\ 0 & g & 0 \end{pmatrix}.$$

By a similarity transformation $A_i \longrightarrow SA_iS^{-1}$ where $S = \text{diagonal}(1, p, pq)$, the parameters of the matrix A_0 are both set equal to 1, (the parameters of A_1 change which we again denote them by g and h .) At this stage no similarity transformation or re-scaling, can reduce the number of parameters, however we note that the matrices A_0 and A_1 act as raising and lowering operators on the 3 dimensional space they act on, (*i.e.* $A_0|i\rangle = |i+1\rangle$, $A_1|i\rangle \propto |i-1\rangle$) and hence the trace of any string of operators $A_{i_1}A_{i_2} \cdots A_{i_{2N}}$ is non-zero only if the number of A_0 and A_1 operators are equal in such a string. This implies first that any such string should be of even length (that is why we have taken a ring of even length), and second that a factor of h^N will be

removed from the numerator and denominator of (4) due to the normalization of the state.

Thus the final matrices which will make a matrix product state with S_z symmetry, will be of the form:

$$A_0 := \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad A_1 := \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & g & 0 \end{pmatrix}. \quad (11)$$

This is all we can go with S_z symmetry and we will in fact make a detailed study of such models in the next section.

What happens if we impose the discrete spin-flip symmetry on the state? This demands that there be a matrix X and a scalar λ such that

$$A_0 = \lambda X A_1 X^{-1}, \quad A_1 = \lambda X A_0 X^{-1}.$$

A short calculation shows that the matrix X which satisfies the above equation is equal to

$$X = \begin{pmatrix} 0 & 0 & 1 \\ 0 & \lambda & 0 \\ \lambda^2 & 0 & 0 \end{pmatrix},$$

where $\lambda^2 = g = 1$. Thus spin-flip symmetry requires that the parameter g be a discrete parameter which we rename as $g = \epsilon$, where $\epsilon = \pm 1$.

It is now found that the parity symmetry imposes no new condition on the parameters, since with the following matrix

$$\Pi = \begin{pmatrix} 0 & 0 & 1 \\ 0 & \sqrt{\epsilon} & 0 \\ \epsilon & 0 & 0 \end{pmatrix},$$

one can verify that $A_i^T = \sqrt{\epsilon} \Pi A_i \Pi^{-1}$. Therefore the final form of the matrices leading to a model with a continuous S_z symmetry plus two discrete parity and spin flip symmetries will be of the form:

$$A_0 := \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad A_1 := \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & \epsilon & 0 \end{pmatrix}. \quad (12)$$

How is the matrix product state (4) with the above matrices related to the states $|\phi_{1,2}\rangle$? We will show in the next section, when we study the generalization of this model, that the matrix product state is equal to $|\phi_1\rangle + |\phi_2\rangle$, that is it is the linear superposition of the ground states which is invariant under translation (with eigenvalue 1). In fact it has been shown that both $|\phi_1\rangle$ and $|\phi_2\rangle$ are ground states and so translation invariant combinations of them, namely $|\Psi_\pm\rangle := |\phi_1\rangle \pm |\phi_2\rangle$, are

also ground states. The point is that only $|\Psi_+\rangle$ has a matrix product representation. It sometimes happens that from a single matrix product state, one can derive the degenerate ground states of a model not all of which have matrix product representations. The Majumdar-Ghosh model is one such case.

Let us also find the Hamiltonian. With the matrices (12) we should solve the equations $\sum_{i,j,k=0}^1 c_{ijk} A_i A_j A_k = 0$. It is readily found that the solution space of this system is spanned by the following four vectors:

$$\begin{aligned} |e_1\rangle &= |000\rangle \\ |e_2\rangle &= |111\rangle \\ |e_3\rangle &= |001\rangle - \epsilon |010\rangle + |100\rangle \\ |e_4\rangle &= |011\rangle - \epsilon |101\rangle + |110\rangle. \end{aligned}$$

These vectors are parity invariant (invariant under left-right reflection) and are mapped to each other under spin-flip transformation ($|0\rangle \rightarrow |1\rangle$, $|1\rangle \rightarrow |0\rangle$). A Hamiltonian with all three symmetries is constructed as:

$$h = J(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2|) + K(|e_3\rangle\langle e_3| + |e_4\rangle\langle e_4|),$$

which when expanded in terms of the spin operators, and embedded into the chain, makes the total Hamiltonian equal to the following:

$$H = \sum_{i=1}^N -K\epsilon\sigma_i \cdot \sigma_{i+1} + \frac{K}{2}\sigma_i \cdot \sigma_{i+2} + \frac{J+(2\epsilon-1)K}{2}\sigma_{i,z}\sigma_{i+1,z} + \frac{J-3K}{4}\sigma_{i,z}\sigma_{i+2,z}.$$

For $\epsilon = 1$ this reduces to

$$H_1 = \sum_{i=1}^{2N} -K\sigma_i \cdot \sigma_{i+1} + \frac{K}{2}\sigma_i \cdot \sigma_{i+2} + \frac{J+K}{2}\sigma_{i,z}\sigma_{i+1,z} + \frac{J-3K}{4}\sigma_{i,z}\sigma_{i+2,z},$$

and for $\epsilon = -1$ reduces to

$$H_{-1} = \sum_{i=1}^{2N} K\sigma_i \cdot \sigma_{i+1} + \frac{K}{2}\sigma_i \cdot \sigma_{i+2} + \frac{J-3K}{4}(2\sigma_{i,z}\sigma_{i+1,z} + \sigma_{i,z}\sigma_{i+2,z}).$$

It is the Hamiltonian H_{-1} which turns into the already familiar Majumdar-Ghosh model (1), by taking $J = 3K$. For general values of J and K it describes the anisotropic Majumdar-Ghosh model, where the anisotropy parameter $\frac{J_z}{J_x = J_y}$ is the same for both the nearest and next-nearest neighbors.

We do not know whether this is already well-known that this model is also exactly solvable. In fact one can check directly that the eigenstates (2) are also eigenstates of the operator

$$H_z := \sum_{i=1}^{2N} 2\sigma_i^z \sigma_{i+1}^z + \sigma_i^z \sigma_{i+2}^z,$$

with eigenvalue $2N$. To see this one needs to invoke the following relations which hold true for any two consecutive singlets S_{12} and S_{34} :

$$\begin{aligned}\sigma_1^z \sigma_2^z S_{1,2} S_{3,4} &= -S_{1,2} S_{3,4} \\ \sigma_1^z \sigma_3^z S_{1,2} S_{3,4} &= U_{1,2} U_{3,4} \\ \sigma_2^z \sigma_3^z S_{1,2} S_{3,4} &= -U_{1,2} U_{3,4},\end{aligned}$$

where $U = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$.

Using these relations one sees that in $H_z |\phi_{1,2}\rangle$ all the terms containing the U terms cancel out and one is left with $H_z |\phi_{1,2}\rangle = -2N |\phi_{1,2}\rangle$.

Putting all these together we find

$$H_{-1} |\phi_{1,2}\rangle = \frac{-J - 3K}{2} N |\phi_{1,2}\rangle.$$

What is the Hamiltonian H_1 ? Does it represent any new model? The answer is negative. To see this we note that by rotating the even-numbered spins around the z axis by an angle of π , under which $\sigma_{2i}^{x,y} \rightarrow -\sigma_{2i}^{x,y}$ and $\sigma_{2i}^z \rightarrow \sigma_{2i}^z$, while keeping the odd-numbered spins intact, the Hamiltonian H_1 is mapped onto H_{-1} .

This transformation will map the states $|\phi_{1,2}\rangle$ onto the states $|\chi_{1,2}\rangle$ where

$$\begin{aligned}|\chi_1\rangle &= U_{1,2} U_{3,4} \cdots U_{2N-1,2N}, \\ |\chi_2\rangle &= U_{2N,1} U_{2,3} \cdots U_{2N-2,2N-1}.\end{aligned}$$

These states are the doubly degenerate ground states of H_1 .

4 Deformation of the Majumdar-Ghosh model

In the last section we have shown how the Majumdar-Ghosh Hamiltonian and its ground states are derived in the matrix product formalism. Let us now relax the condition of parity symmetry, which automatically removes also the spin flip symmetry. Then the matrices will be of the form (11), which still have the continuous symmetry of rotation around the z axis. It is now easily verified that the solution space of the system of equations (8) with $k = 3$ is spanned by the following four vectors:

$$\begin{aligned}|e_1\rangle &= |000\rangle \\ |e_2\rangle &= |111\rangle \\ |e_3\rangle &= |001\rangle - g|010\rangle + g^2|100\rangle \\ |e_4\rangle &= |011\rangle - g|101\rangle + g^2|110\rangle.\end{aligned}$$

The most general local Hamiltonian having the matrix product state as its ground state is now given by

$$h = J_1 |e_1\rangle\langle e_1| + J_2 |e_2\rangle\langle e_2| + J_3 |e_3\rangle\langle e_3| + J_4 |e_4\rangle\langle e_4|.$$

Rewriting this in terms of spin operators we find after some rather lengthy calculations the following form of the final Hamiltonian

$$H = \frac{1}{8} \sum_{i=1}^N K_1 \sigma_i \cdot \sigma_{i+1} + K_2 \sigma_i \cdot \sigma_{i+2} + K_3 \sigma_i^z \sigma_{i+1}^z + K_4 \sigma_i^z \sigma_{i+2}^z + K_5 \sigma_i^z + K_6 \sigma_i^z \sigma_{i+1}^z \sigma_{i+2}^z + K_7 \sigma_i^z \sigma_{i+1} \sigma_{i+2} + K_8 \sigma_i \cdot \sigma_{i+1} \sigma_{i+2}^z + K_9 \sigma_i \cdot \sigma_{i+1}^z \sigma_{i+2}, \quad (13)$$

where the couplings are

$$\begin{aligned} K_1 &= -2g(1+g^2)(J_3 + J_4) \\ K_2 &= 2g^2(J_3 + J_4) \\ K_3 &= 2(J_1 + J_2) + 2(J_3 + J_4)(g - g^2 + g^3) \\ K_4 &= J_1 + J_2 - (J_3 + J_4)(1 + g^2 + g^4) \\ K_5 &= 3(J_1 - J_2) + (J_3 - J_4)(1 + g^2 + g^4) \\ K_6 &= J_1 - J_2 - (J_3 - J_4)(1 - g + g^2)^2 \\ K_7 &= -2gJ_3 + 2g^3J_4 \\ K_8 &= -2g^3J_3 + 2gJ_4 \\ K_9 &= 2g^2(J_3 - J_4). \end{aligned}$$

This is a 5-parameter family of models with nearest neighbor and next-nearest neighbor interactions, whose ground state can be written down exactly. We will show that with the couplings as above, this model has a doubly degenerate ground state, each of which has a simple product structure of dimers, like the one given in (2).

Note that the Hamiltonian (13) will reduce to H_{-1} when we restrict the parameters as follows

$$g = -1, J_1 = J_2 = J, J_3 = J_4 = K$$

and to (1) when we further set $J = 3K$.

4.1 Structure of the matrix product state

The matrix product state (11) has a simple structure. We prove the following theorem:

Theorem: The matrix product state (4) constructed from the matrices (11) which is a ground state of (13) has the following structure. Define a state

$$S(g) := g|01\rangle + |10\rangle,$$

$$\begin{aligned} |\phi_1(g)\rangle &= S_{1,2}(g)S_{3,4}(g)S_{5,6}(g) \cdots S_{2N-1,2N}(g) \\ |\phi_2(g)\rangle &= S_{2N,1}(g)S_{2,3}(g)S_{4,5}(g) \cdots S_{2N-2,2N-1}(g), \end{aligned} \quad (14)$$

that is $|\phi_2(g)\rangle = T|\phi_1(g)\rangle$, where T is the translation operator along the chain by one lattice unit. Then we have

$$|\Psi(g)\rangle = |\phi_1(g)\rangle + |\phi_2(g)\rangle.$$

Proof: Consider the matrix product state $|\Psi(g)\rangle = \sum \Psi_{i_1 i_2 \dots i_{2N}} |i_1 i_2 \dots i_{2N}\rangle$. The amplitudes $\Psi_{i_1 i_2 \dots i_{2N}}$ are non-vanishing only when

- i) the number of 0 indices and 1 indices are equal (in view of the fact that the matrices A_0 and A_1 are raising and lowering operators), ii) no three consecutive indices are 0 or 1, (since $A_0^3 = A_1^3 = 0$), and iii) no substrings of the types $\dots 11011 \dots$ or $\dots 00100 \dots$ appear in the indices, (since $A_1^2 A_0 A_1^2 = A_0^2 A_1 A_0^2 = 0$.)

Let us define the compact notations $\mathbf{0} := 01$ and $\mathbf{1} := 10$. In view of the above three properties, we can divide the set of states $|i_1, i_2, \dots, i_{2N}\rangle$ into two types, type 1, which are states of the form $|\mathbf{00110}\rangle = |0101101001\rangle$, that is, strings of $\mathbf{0}$'s and $\mathbf{1}$'s in arbitrary order, and type 2, which are transformed to the above type by a one-unit cyclic translation like $|1010110100\rangle$. There is a one to one correspondence between these two types of states and hence the state $|\Psi\rangle$ can be divided in two parts, depending on the type of basis states $|\Psi(g)\rangle = |\phi_1(g)\rangle + |\phi_2(g)\rangle$, where

$$\phi_1(g) = \sum_{\alpha_1, \alpha_2, \dots, \alpha_N = \mathbf{0}, \mathbf{1}} \phi_{\alpha_1 \alpha_2 \dots \alpha_N} |\alpha_1 \alpha_2 \dots \alpha_N\rangle$$

and $|\phi_2(g)\rangle = T|\phi_1(g)\rangle$. We now note that

$$A_{\mathbf{0}} \equiv A_0 A_1 = \begin{pmatrix} 1 & \\ & g \end{pmatrix} \quad A_{\mathbf{1}} \equiv A_1 A_0 = \begin{pmatrix} & 1 \\ 1 & g \end{pmatrix}. \quad (15)$$

This means that $A_{\mathbf{0}}$ and $A_{\mathbf{1}}$ commute with each other, which immediately implies that $|\phi_1(g)\rangle$ is a product state, i.e.

$$|\phi_1(g)\rangle = \sum_{m=0}^N \text{tr}(A_{\mathbf{0}}^m A_{\mathbf{1}}^{N-m}) |\mathbf{0}^m \mathbf{1}^{N-m}\rangle = \sum_{m=0}^N g^m |\mathbf{0}^m \mathbf{1}^{N-m}\rangle = (g|\mathbf{0}\rangle + |\mathbf{1}\rangle)^{\otimes N},$$

where $|\mathbf{0}^m \mathbf{1}^{N-m}\rangle$ denotes a uniform superposition of states each of which has m $\mathbf{0}$'s and $N - m$ $\mathbf{1}$'s, in different positions. This completes the proof.

Are the two individual states $|\phi_1(g)\rangle$ and $|\phi_2(g)\rangle$ the ground states of H ? There are supports for thinking so. First we have checked this for low values of system size N and second we know that as $g \rightarrow -1$, these states approach the states of Majumdar-Ghosh (2) which are known to be ground states of the Hamiltonian H_{-1} . Therefore we can make two linear combinations of these ground states, namely $|\Psi_+(g)\rangle := |\phi_1(g)\rangle + |\phi_2(g)\rangle$ which has a matrix product representation and $|\Psi_-(g)\rangle := |\phi_1(g)\rangle - |\phi_2(g)\rangle$ which does not have such a representation. In the next subsection we calculate the correlation functions on these translation invariant states and they again approach the ones calculated in [12] in the limit $g = -1$ and $N \rightarrow \infty$. For our future reference we need the following easily verified properties:

$$\langle \phi_1(g) | \phi_1(g) \rangle = \langle \phi_2(g) | \phi_2(g) \rangle = (1 + g^2)^N \quad \langle \phi_1(g) | \phi_2(g) \rangle = \langle \phi_2(g) | \phi_1(g) \rangle = 2g^N.$$

4.2 Correlation functions

In the Majumdar-Ghosh model both the ground states (2) have anti-ferromagnetic order and $\langle \sigma_i^{x,y,z} \rangle = 0$. This is clear from the fact that the states (2) are product of singlets on adjacent sites. In our model, the states are no longer singlets and while there is no magnetic order present, the staggered magnetization is non-vanishing. Consider the states $|\phi_1(g)\rangle$, and $|\phi_2(g)\rangle$. In view of their simple product structure, it is readily seen that

$$\langle \phi_1(g) | \sigma_1^z | \phi_1(g) \rangle = -\langle \phi_1(g) | \sigma_2^z | \phi_1(g) \rangle = \langle S_{12} | \sigma_1^z | S_{12} \rangle = \frac{1-g^2}{1+g^2}, \quad (16)$$

and

$$\langle \phi_2(g) | \sigma_1^z | \phi_2(g) \rangle = -\langle \phi_2(g) | \sigma_2^z | \phi_2(g) \rangle = \langle S_{2N,1} | \sigma_1^z | S_{2N,1} \rangle = \frac{g^2-1}{1+g^2}. \quad (17)$$

This means that the value of staggered magnetization defined as

$$(m_s)_{\phi_i} := \frac{1}{2N} \sum_{i=1}^N \langle \phi_i | \sigma_{z,2i-1} - \sigma_{z,2i} | \phi_i \rangle$$

is non-zero in these two states, i.e.

$$(m_s)_{\phi_1} = \frac{1-g^2}{1+g^2}, \quad (m_s)_{\phi_2} = \frac{g^2-1}{1+g^2}.$$

However there is no staggered magnetization in the translation invariant states $|\Psi_{\pm}\rangle$. To see this we can calculate σ_1^z for the state $|\Psi_{+}\rangle = |\phi_1(g)\rangle + |\phi_2(g)\rangle$, either by using the matrix product formula (9) or by a direct calculation in which we use (16), (17) and

$$\langle \Psi_{\pm} | O | \Psi_{\pm} \rangle = \frac{\langle \phi_1 | O | \phi_1 \rangle + \langle \phi_2 | O | \phi_2 \rangle \pm 2\langle \phi_1 | O | \phi_2 \rangle}{2\langle \phi_1 | \phi_1 \rangle \pm 2\langle \phi_1 | \phi_2 \rangle}, \quad (18)$$

in which O is any operator and we have abbreviated $|\phi_i(g)\rangle$ to $|\phi_i\rangle$ and used the fact that $\langle \phi_1 | \phi_1 \rangle = \langle \phi_2 | \phi_2 \rangle$ to simplify terms in the denominator. For this direct calculation, the only new quantity which is needed is $\langle \phi_1(g) | \sigma_1^z | \phi_2(g) \rangle$. We know that all the states in the expansion of $|\phi_1(g)\rangle$ and $|\phi_2(g)\rangle$ are different from each other except the states $|\mathbf{010}\cdots\mathbf{1}\rangle$ and $|\mathbf{101}\cdots\mathbf{0}\rangle$ which are common to both and transformed into each other by the action of the translation operator T . So we find

$$\langle \phi_1(g) | \sigma_1^z | \phi_2(g) \rangle = (g^n \langle \mathbf{01}\cdots\mathbf{1} | + \langle \mathbf{10}\cdots\mathbf{0} |) | \sigma_1^z | (g^n | \mathbf{10}\cdots\mathbf{0} \rangle + | \mathbf{01}\cdots\mathbf{1} \rangle) = 0, \quad (19)$$

implying that there is no staggered magnetization in $|\Psi_{\pm}\rangle$.

The two point functions can also be calculated along similar lines. We point out only the general method. The product nature of $|\phi_1\rangle$ and $|\phi_2\rangle$, formula (18) and the reasoning used above for the calculation of the cross term $\langle \phi_1(g) | \sigma_1^z \sigma_r^z | \phi_2(g) \rangle$ facilitate calculations of $\langle \sigma_1^z \sigma_r^z \rangle_{\pm}$. However the cross term $\langle \phi_1(g) | \sigma_1^x \sigma_r^x | \phi_2(g) \rangle$ is hard to calculate in this way. Instead we calculate $\langle \sigma_1^x \sigma_r^x \rangle_{+}$ (i.e. for the matrix product

state $|\Psi_+\rangle$) from (10) and infer the cross term from its result. We then use this cross term for determining the correlation $\langle\sigma_1^x\sigma_r^x\rangle_-$. The reader can verify these results by direct calculation for chains of small size. The interesting point is that all the correlation functions can be expressed in terms of a variable $u := g + \frac{1}{g}$ which is invariant under the interchange of $g \rightarrow \frac{1}{g}$. The results are:

$$\langle\sigma_1^z\sigma_2^z\rangle_{\pm} = \frac{-2 \pm u^N(2u^{-2}-1)}{2 \pm u^N}, \quad \langle\sigma_1^z\sigma_{r>2}^z\rangle = (-1)^r \frac{-2 \pm u^N(4u^{-2}-1)}{2 \pm u^N},$$

and

$$\langle\sigma_1^n\sigma_2^n\rangle_{\pm} = \frac{u \pm u^{N-1}}{2 \pm u^N}, \quad \langle\sigma_1^n\sigma_{r>2}^n\rangle = \frac{2\delta_{r,odd} + \delta_{r,even}u}{2 \pm u^N}.$$

It can be verified that these correlation functions reduce to (3) at the point $g = -1$ ($u = -2$), after we take the thermodynamic limit ($N \rightarrow \infty$).

5 Discussion

We have constructed a 5-parameter family of spin-Hamiltonians with nearest and next nearest neighbor interactions and have found their exact ground states. The ground states, depend on only one of these parameters, are doubly degenerate and have a very simple structure. They are product of entangled states (dimers) on adjacent spins. We have also calculated the one and the two point functions in closed analytic form both for finite size of the chain and in the thermodynamic limit. The dimerized ground states show staggered magnetization, but the translation-invariant combinations of these states have no staggered magnetization.

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